



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:04 PM UTC

PDB ID : 4G1U / pdb_00004g1u
Title : X-ray structure of the bacterial heme transporter HmuUV from Yersinia pestis
Authors : Woo, J.-S.; Goetz, B.A.; Zeltina, A.; Locher, K.P.
Deposited on : 2012-07-11
Resolution : 3.01 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

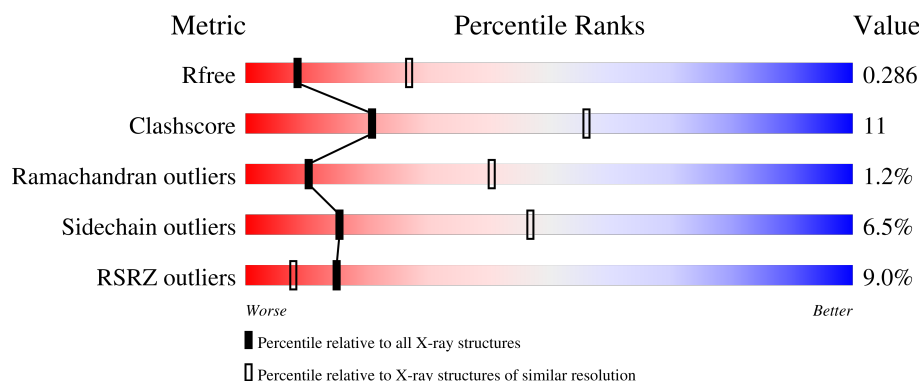
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	357	
1	B	357	
2	C	266	
2	D	266	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8499 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemin transport system permease protein hmuU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2209	1451	380	365	13			
1	B	297	Total	C	N	O	S	0	0	0
			2209	1451	380	365	13			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q56992
A	-21	GLY	-	expression tag	UNP Q56992
A	-20	HIS	-	expression tag	UNP Q56992
A	-19	HIS	-	expression tag	UNP Q56992
A	-18	HIS	-	expression tag	UNP Q56992
A	-17	HIS	-	expression tag	UNP Q56992
A	-16	HIS	-	expression tag	UNP Q56992
A	-15	HIS	-	expression tag	UNP Q56992
A	-14	HIS	-	expression tag	UNP Q56992
A	-13	HIS	-	expression tag	UNP Q56992
A	-12	HIS	-	expression tag	UNP Q56992
A	-11	HIS	-	expression tag	UNP Q56992
A	-10	SER	-	expression tag	UNP Q56992
A	-9	SER	-	expression tag	UNP Q56992
A	-8	GLY	-	expression tag	UNP Q56992
A	-7	GLU	-	expression tag	UNP Q56992
A	-6	ASN	-	expression tag	UNP Q56992
A	-5	LEU	-	expression tag	UNP Q56992
A	-4	TYR	-	expression tag	UNP Q56992
A	-3	PHE	-	expression tag	UNP Q56992
A	-2	GLN	-	expression tag	UNP Q56992
A	-1	GLY	-	expression tag	UNP Q56992
A	0	HIS	-	expression tag	UNP Q56992
B	-22	MET	-	expression tag	UNP Q56992
B	-21	GLY	-	expression tag	UNP Q56992

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	expression tag	UNP Q56992
B	-19	HIS	-	expression tag	UNP Q56992
B	-18	HIS	-	expression tag	UNP Q56992
B	-17	HIS	-	expression tag	UNP Q56992
B	-16	HIS	-	expression tag	UNP Q56992
B	-15	HIS	-	expression tag	UNP Q56992
B	-14	HIS	-	expression tag	UNP Q56992
B	-13	HIS	-	expression tag	UNP Q56992
B	-12	HIS	-	expression tag	UNP Q56992
B	-11	HIS	-	expression tag	UNP Q56992
B	-10	SER	-	expression tag	UNP Q56992
B	-9	SER	-	expression tag	UNP Q56992
B	-8	GLY	-	expression tag	UNP Q56992
B	-7	GLU	-	expression tag	UNP Q56992
B	-6	ASN	-	expression tag	UNP Q56992
B	-5	LEU	-	expression tag	UNP Q56992
B	-4	TYR	-	expression tag	UNP Q56992
B	-3	PHE	-	expression tag	UNP Q56992
B	-2	GLN	-	expression tag	UNP Q56992
B	-1	GLY	-	expression tag	UNP Q56992
B	0	HIS	-	expression tag	UNP Q56992

- Molecule 2 is a protein called Hemin import ATP-binding protein HmuV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	262	Total	C	N	O	S	0	0	0
			2052	1294	374	374	10			
2	D	257	Total	C	N	O	S	0	0	0
			2019	1272	369	368	10			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

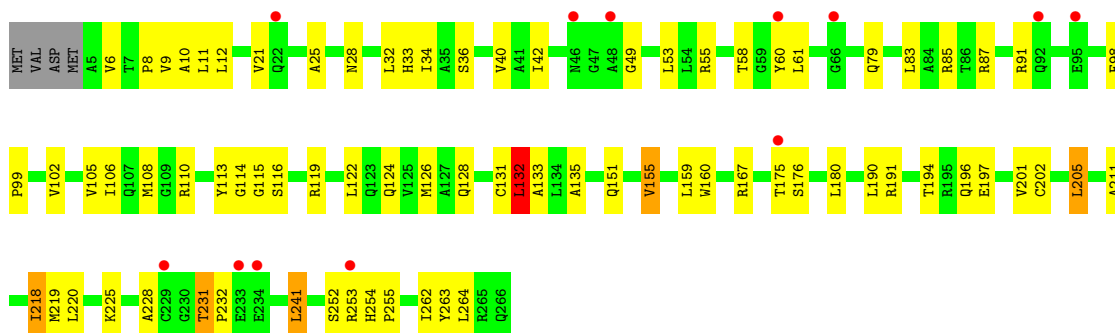


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

GLN
ARG
GLU
GLN
ARG
SER
GLY

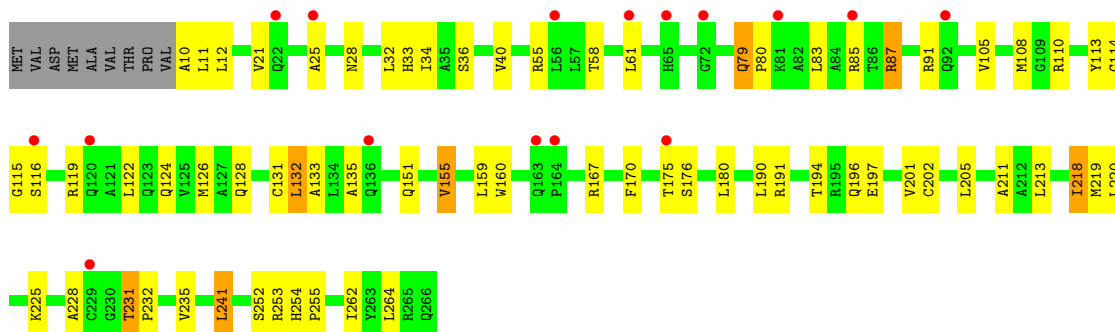
• Molecule 2: Hemin import ATP-binding protein HmuV

Chain C:  5% 69% 27%



• Molecule 2: Hemin import ATP-binding protein HmuV

Chain D:  6% 70% 24%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.87Å 101.23Å 105.21Å 90.00° 91.30° 90.00°	Depositor
Resolution (Å)	29.77 – 3.01 29.77 – 3.01	Depositor EDS
% Data completeness (in resolution range)	88.4 (29.77-3.01) 88.3 (29.77-3.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.37 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.7.2_869	Depositor
R, R_{free}	0.263 , 0.295 0.258 , 0.286	Depositor DCC
R_{free} test set	1971 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	72.6	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.004 for -h,-l,-k 0.000 for -l,k,h 0.000 for -k,-h,-l 0.000 for k,h,-l 0.000 for k,l,h 0.000 for l,h,k 0.000 for l,-h,-k 0.000 for -k,-l,h 0.000 for h,-k,-l 0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8499	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.49	0/2247	0.89	6/3061 (0.2%)
1	B	0.47	0/2247	0.89	8/3061 (0.3%)
2	C	0.43	0/2095	0.79	2/2854 (0.1%)
2	D	0.35	0/2061	0.77	2/2805 (0.1%)
All	All	0.44	0/8650	0.84	18/11781 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	HIS	N-CA-C	-8.16	102.78	112.89
1	B	86	ASP	CA-C-N	6.93	128.50	119.84
1	B	86	ASP	C-N-CA	6.93	128.50	119.84
1	B	303	ALA	CA-C-N	6.56	128.04	119.84
1	B	303	ALA	C-N-CA	6.56	128.04	119.84
1	A	303	ALA	CA-C-N	6.51	127.98	119.84
1	A	303	ALA	C-N-CA	6.51	127.98	119.84
1	A	86	ASP	CA-C-N	6.24	127.64	119.84
1	A	86	ASP	C-N-CA	6.24	127.64	119.84
2	D	79	GLN	CA-C-N	6.10	126.28	119.32
2	D	79	GLN	C-N-CA	6.10	126.28	119.32
2	C	79	GLN	CA-C-N	5.96	126.11	119.32
2	C	79	GLN	C-N-CA	5.96	126.11	119.32
1	B	318	GLY	CA-C-N	5.62	125.71	119.87
1	B	318	GLY	C-N-CA	5.62	125.71	119.87
1	A	318	GLY	CA-C-N	5.59	125.69	119.87
1	A	318	GLY	C-N-CA	5.59	125.69	119.87
1	B	90	LEU	N-CA-C	-5.03	107.15	113.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2209	0	2380	64	0
1	B	2209	0	2380	61	0
2	C	2052	0	2060	44	0
2	D	2019	0	2023	42	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
All	All	8499	0	8843	193	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (193) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:167:ARG:NH2	2:C:197:GLU:OE1	2.11	0.83
2:D:167:ARG:NH2	2:D:197:GLU:OE1	2.12	0.81
2:C:176:SER:HB2	2:D:176:SER:HB2	1.69	0.75
1:A:86:ASP:OD1	1:A:88:GLY:N	2.23	0.72
2:C:252:SER:HB2	2:D:255:PRO:HG3	1.74	0.69
1:A:79:LEU:O	1:A:139:ARG:NH2	2.28	0.67
1:B:79:LEU:O	1:B:139:ARG:NH2	2.28	0.66
1:A:76:MET:HE1	1:A:247:ILE:HD11	1.78	0.65
1:A:146:ALA:HB2	1:B:146:ALA:HB2	1.76	0.65
2:D:131:CYS:O	2:D:133:ALA:N	2.27	0.64
2:C:131:CYS:O	2:C:133:ALA:N	2.32	0.63
1:A:58:ARG:HH12	1:A:187:GLY:HA2	1.62	0.63
2:D:241:LEU:HD11	2:D:262:ILE:HG12	1.81	0.62
2:C:10:ALA:HB3	2:C:36:SER:HB2	1.82	0.62
1:B:86:ASP:OD1	1:B:88:GLY:N	2.32	0.62
2:C:241:LEU:HD11	2:C:262:ILE:HG12	1.81	0.62
1:B:58:ARG:HH12	1:B:187:GLY:HA2	1.63	0.62
2:C:124:GLN:OE1	2:C:160:TRP:NE1	2.32	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LEU:HA	1:B:117:TYR:HB2	1.83	0.61
1:A:53:ASN:HA	1:A:191:TRP:HE1	1.66	0.60
2:C:113:TYR:O	2:C:115:GLY:N	2.33	0.60
2:D:10:ALA:HB3	2:D:36:SER:HB2	1.83	0.60
1:A:114:LEU:HA	1:A:117:TYR:HB2	1.83	0.59
1:A:276:HIS:HA	1:A:279:LEU:HB3	1.84	0.59
2:D:113:TYR:O	2:D:115:GLY:N	2.36	0.58
2:C:49:GLY:HA2	3:C:301:PO4:O3	2.03	0.57
1:B:127:SER:O	1:B:131:SER:HB2	2.04	0.57
2:D:124:GLN:OE1	2:D:160:TRP:NE1	2.32	0.57
1:A:76:MET:HE3	1:A:87:PRO:HD3	1.85	0.57
1:A:90:LEU:HD13	1:A:134:ILE:HG21	1.87	0.56
1:B:53:ASN:HA	1:B:191:TRP:HE1	1.69	0.56
1:B:220:LEU:HD11	2:C:108:MET:HG2	1.87	0.56
2:C:110:ARG:CZ	2:C:113:TYR:HD2	2.19	0.56
1:A:302:VAL:HG21	1:B:169:ILE:HD12	1.88	0.56
2:D:231:THR:HG22	2:D:232:PRO:HD2	1.88	0.56
2:D:254:HIS:HD2	2:D:255:PRO:HD2	1.70	0.55
1:B:18:LEU:HD11	1:B:63:VAL:HG22	1.88	0.55
1:A:326:LEU:HD13	1:B:137:LEU:HD21	1.89	0.55
1:B:276:HIS:HA	1:B:279:LEU:HB3	1.89	0.54
2:C:254:HIS:HD2	2:C:255:PRO:HD2	1.71	0.54
1:B:217:LEU:HD23	2:C:108:MET:HG3	1.89	0.54
2:D:110:ARG:CZ	2:D:113:TYR:HD2	2.21	0.54
1:A:18:LEU:HD11	1:A:63:VAL:HG22	1.91	0.53
1:A:127:SER:O	1:A:131:SER:HB2	2.09	0.53
1:A:130:ILE:HD13	1:A:155:ILE:HD13	1.90	0.53
2:C:190:LEU:HB3	2:C:201:VAL:HG21	1.91	0.53
1:B:90:LEU:HD13	1:B:134:ILE:HG21	1.91	0.53
2:C:231:THR:HG22	2:C:232:PRO:HD2	1.90	0.53
1:A:209:LEU:HA	1:A:280:LEU:HD13	1.90	0.53
1:B:68:ALA:HB2	1:B:201:ILE:HD13	1.91	0.53
1:A:217:LEU:HD23	2:D:108:MET:HG3	1.91	0.52
1:B:130:ILE:HD13	1:B:155:ILE:HD13	1.90	0.52
2:D:190:LEU:HB3	2:D:201:VAL:HG21	1.89	0.52
2:D:252:SER:OG	2:D:253:ARG:N	2.43	0.52
1:B:139:ARG:CZ	1:B:236:LYS:HE2	2.39	0.52
2:D:211:ALA:HB1	2:D:218:ILE:HD11	1.92	0.52
1:B:209:LEU:HA	1:B:280:LEU:HD13	1.91	0.52
1:A:48:TRP:C	1:A:50:ILE:H	2.18	0.52
1:A:223:GLU:HG2	1:A:227:TYR:CE1	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:34:ILE:HD13	2:C:202:CYS:HB2	1.93	0.51
2:C:220:LEU:HB3	2:C:228:ALA:HB3	1.93	0.51
1:A:139:ARG:CZ	1:A:236:LYS:HE2	2.39	0.51
2:D:105:VAL:HA	2:D:108:MET:HE2	1.92	0.51
2:C:159:LEU:HD22	2:C:167:ARG:HB3	1.93	0.51
1:A:99:CYS:O	1:A:103:ILE:HG12	2.10	0.50
1:A:68:ALA:HA	1:A:246:LEU:HD22	1.94	0.50
1:A:165:VAL:O	1:A:169:ILE:HG12	2.12	0.50
1:B:146:ALA:O	1:B:150:LEU:HG	2.11	0.50
1:B:165:VAL:O	1:B:169:ILE:HG12	2.11	0.50
2:D:34:ILE:HD13	2:D:202:CYS:HB2	1.94	0.50
1:A:220:LEU:HD11	2:D:108:MET:HG2	1.94	0.50
1:A:146:ALA:O	1:A:150:LEU:HG	2.12	0.50
1:B:76:MET:HE1	1:B:247:ILE:HD11	1.92	0.49
2:C:105:VAL:HA	2:C:108:MET:HE2	1.93	0.49
1:B:99:CYS:O	1:B:103:ILE:HG12	2.12	0.49
2:D:220:LEU:HB3	2:D:228:ALA:HB3	1.94	0.49
1:A:68:ALA:HB2	1:A:201:ILE:HD13	1.93	0.49
2:C:252:SER:OG	2:C:253:ARG:N	2.43	0.49
1:B:223:GLU:HG2	1:B:227:TYR:CE1	2.48	0.49
2:C:263:TYR:HD2	2:D:254:HIS:HE2	1.60	0.48
2:C:85:ARG:HG2	2:C:113:TYR:HE1	1.78	0.48
2:D:159:LEU:HD22	2:D:167:ARG:HB3	1.94	0.48
2:D:85:ARG:HG2	2:D:113:TYR:HE1	1.78	0.48
2:C:151:GLN:O	2:C:155:VAL:HG12	2.14	0.47
2:C:211:ALA:HB1	2:C:218:ILE:HD11	1.94	0.47
2:C:126:MET:HE1	2:C:135:ALA:HB2	1.96	0.47
1:A:197:ALA:HB2	1:A:253:VAL:HG21	1.97	0.47
1:B:227:TYR:OH	2:C:58:THR:HG21	2.14	0.47
1:B:5:VAL:HG11	1:B:10:MET:HE2	1.96	0.47
1:B:177:GLN:NE2	1:B:188:GLN:OE1	2.47	0.47
1:B:76:MET:HG3	1:B:80:PHE:CE1	2.50	0.47
1:B:201:ILE:HA	1:B:204:THR:HG22	1.97	0.47
2:C:124:GLN:HG2	2:C:128:GLN:HE21	1.78	0.47
1:B:76:MET:HE3	1:B:87:PRO:HD3	1.96	0.46
1:B:264:VAL:HG21	1:B:286:GLY:C	2.40	0.46
2:D:151:GLN:O	2:D:155:VAL:HG12	2.15	0.46
1:B:81:ARG:HH12	1:B:139:ARG:HH12	1.64	0.46
1:A:297:LEU:O	1:A:301:LEU:HB2	2.16	0.46
2:C:55:ARG:NH2	2:C:91:ARG:HH21	2.14	0.46
1:A:177:GLN:NE2	1:A:188:GLN:OE1	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:HD21	2:D:108:MET:HE3	1.98	0.46
1:A:264:VAL:HG21	1:A:286:GLY:C	2.40	0.46
1:A:5:VAL:HG11	1:A:10:MET:HE2	1.99	0.45
1:A:264:VAL:HG12	1:A:265:PRO:HD3	1.97	0.45
2:D:126:MET:HE1	2:D:135:ALA:HB2	1.97	0.45
1:A:58:ARG:NH1	1:A:187:GLY:HA2	2.30	0.45
1:B:68:ALA:HA	1:B:246:LEU:HD22	1.98	0.45
1:B:95:GLY:HA3	1:B:130:ILE:HD12	1.97	0.45
1:A:76:MET:HG3	1:A:80:PHE:CE1	2.52	0.45
1:A:95:GLY:HA3	1:A:130:ILE:HD12	1.98	0.45
1:A:139:ARG:NH1	1:A:222:ASP:OD1	2.50	0.45
1:A:201:ILE:HA	1:A:204:THR:HG22	1.98	0.45
1:B:6:GLN:HG3	1:B:7:PRO:HD2	1.99	0.45
1:A:61:LEU:HD23	1:A:186:LEU:HD22	1.99	0.45
1:A:81:ARG:HH12	1:A:139:ARG:HH12	1.64	0.45
2:D:28:ASN:HB3	2:D:225:LYS:HG2	1.99	0.45
1:B:139:ARG:NH1	1:B:222:ASP:OD1	2.49	0.45
1:B:149:LEU:O	1:B:153:ILE:HG13	2.17	0.45
1:B:297:LEU:O	1:B:301:LEU:HB2	2.17	0.45
2:C:205:LEU:HD13	2:C:211:ALA:HB2	1.98	0.45
1:A:149:LEU:O	1:A:153:ILE:HG13	2.16	0.44
1:A:201:ILE:O	1:A:204:THR:HG22	2.17	0.44
2:D:124:GLN:HG2	2:D:128:GLN:HE21	1.81	0.44
1:A:302:VAL:HG21	1:B:169:ILE:CD1	2.47	0.44
1:A:6:GLN:HG3	1:A:7:PRO:HD2	2.00	0.44
2:C:6:VAL:O	2:C:8:PRO:HD3	2.18	0.44
2:C:32:LEU:HB3	2:C:219:MET:HE1	2.00	0.44
2:C:32:LEU:CB	2:C:219:MET:HE1	2.47	0.44
1:A:262:LEU:HD21	1:A:321:PHE:CD1	2.52	0.44
1:B:264:VAL:HG12	1:B:265:PRO:HD3	1.98	0.44
2:D:32:LEU:CB	2:D:219:MET:HE1	2.48	0.44
1:B:100:VAL:O	1:B:104:ILE:HG23	2.18	0.44
1:B:116:LEU:O	1:B:120:MET:HG2	2.17	0.44
1:B:197:ALA:HB2	1:B:253:VAL:HG21	2.00	0.44
2:C:102:VAL:O	2:C:106:ILE:HG13	2.18	0.44
1:B:58:ARG:NH1	1:B:187:GLY:HA2	2.31	0.43
1:B:262:LEU:HD21	1:B:321:PHE:CD1	2.53	0.43
2:C:28:ASN:HB3	2:C:225:LYS:HG2	1.99	0.43
1:A:116:LEU:O	1:A:120:MET:HG2	2.18	0.43
1:A:100:VAL:O	1:A:104:ILE:HG23	2.19	0.43
1:B:86:ASP:HA	1:B:87:PRO:HD2	1.75	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:ARG:HA	2:D:58:THR:HG22	2.01	0.43
2:D:219:MET:HE2	2:D:219:MET:HB3	1.88	0.43
1:B:28:MET:HE1	1:B:300:THR:HG21	2.01	0.43
1:A:312:LEU:HD23	1:A:312:LEU:HA	1.78	0.43
1:B:220:LEU:HD21	2:C:108:MET:HE3	2.00	0.43
1:B:237:LEU:HD23	1:B:237:LEU:HA	1.85	0.43
1:A:130:ILE:HD13	1:A:155:ILE:HG21	2.01	0.42
1:A:10:MET:HE3	1:A:271:ARG:HB3	2.01	0.42
1:A:89:LEU:HA	1:A:89:LEU:HD12	1.80	0.42
2:D:87:ARG:HG3	2:D:170:PHE:HE1	1.84	0.42
1:B:70:ALA:HB2	1:B:287:GLY:HA3	2.00	0.42
2:D:55:ARG:NH2	2:D:91:ARG:HH21	2.16	0.42
1:A:70:ALA:HB2	1:A:287:GLY:HA3	2.02	0.42
2:D:32:LEU:HB3	2:D:219:MET:HE1	2.01	0.42
1:B:130:ILE:HD13	1:B:155:ILE:HG21	2.01	0.42
2:C:12:LEU:O	2:C:33:HIS:HA	2.19	0.42
1:A:76:MET:HB2	1:A:76:MET:HE2	1.64	0.42
2:D:12:LEU:O	2:D:33:HIS:HA	2.20	0.42
1:A:320:TYR:O	1:A:323:TRP:HB3	2.20	0.42
1:B:10:MET:HE3	1:B:271:ARG:HB3	2.02	0.42
2:D:55:ARG:HB3	2:D:61:LEU:HG	2.02	0.42
1:A:16:ILE:O	1:A:20:ILE:HG12	2.20	0.42
1:A:86:ASP:HA	1:A:87:PRO:HD2	1.75	0.42
1:B:16:ILE:O	1:B:20:ILE:HG12	2.19	0.42
2:D:180:LEU:HD23	2:D:180:LEU:HA	1.83	0.42
1:B:135:PHE:HZ	1:B:236:LYS:HD3	1.84	0.41
2:C:264:LEU:O	2:D:213:LEU:HD21	2.19	0.41
2:C:132:LEU:HD12	2:C:132:LEU:HA	1.87	0.41
2:C:191:ARG:O	2:C:194:THR:HB	2.20	0.41
2:D:253:ARG:HD3	2:D:253:ARG:HA	1.94	0.41
1:A:76:MET:CE	1:A:247:ILE:HD11	2.48	0.41
1:A:135:PHE:HZ	1:A:236:LYS:HD3	1.85	0.41
1:A:215:LEU:HD22	1:A:276:HIS:CD2	2.55	0.41
1:B:201:ILE:O	1:B:204:THR:HG22	2.21	0.41
2:C:180:LEU:HD13	2:D:264:LEU:HD21	2.01	0.41
1:A:136:THR:HG23	1:A:140:TRP:HD1	1.86	0.41
1:A:303:ALA:HB1	1:A:304:PRO:HD2	2.03	0.41
1:B:61:LEU:HD23	1:B:186:LEU:HD22	2.03	0.41
2:D:228:ALA:HB1	2:D:235:VAL:HG22	2.02	0.41
1:A:207:LEU:HD23	1:A:207:LEU:HA	1.72	0.40
2:C:98:PHE:HA	2:C:99:PRO:HD3	1.88	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:191:ARG:O	2:D:194:THR:HB	2.21	0.40
1:B:207:LEU:HA	1:B:207:LEU:HD23	1.75	0.40
2:C:42:ILE:HD12	2:C:53:LEU:HD23	2.03	0.40
2:D:79:GLN:HA	2:D:80:PRO:HD3	1.94	0.40
1:A:212:ALA:HB2	1:A:280:LEU:HD12	2.04	0.40
1:B:267:LEU:HD23	1:B:267:LEU:HA	1.87	0.40
1:A:89:LEU:HD11	1:B:153:ILE:HG21	2.02	0.40
1:B:26:ALA:HB1	1:B:51:TRP:CZ2	2.56	0.40
1:B:77:GLN:HA	1:B:85:ALA:HB3	2.04	0.40
1:B:223:GLU:HG3	2:C:60:TYR:CE1	2.57	0.40
2:C:55:ARG:HB3	2:C:61:LEU:HG	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	291/357 (82%)	271 (93%)	17 (6%)	3 (1%)	12	45
1	B	291/357 (82%)	272 (94%)	17 (6%)	2 (1%)	18	53
2	C	260/266 (98%)	239 (92%)	17 (6%)	4 (2%)	8	35
2	D	255/266 (96%)	233 (91%)	18 (7%)	4 (2%)	7	34
All	All	1097/1246 (88%)	1015 (92%)	69 (6%)	13 (1%)	10	40

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	PRO
1	B	304	PRO
2	C	114	GLY
2	D	114	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	146	ALA
2	C	25	ALA
2	D	25	ALA
1	A	146	ALA
2	C	132	LEU
2	C	196	GLN
2	D	132	LEU
2	D	196	GLN
1	A	318	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	231/283 (82%)	217 (94%)	14 (6%)	17	49
1	B	231/283 (82%)	218 (94%)	13 (6%)	19	52
2	C	219/223 (98%)	203 (93%)	16 (7%)	13	42
2	D	215/223 (96%)	200 (93%)	15 (7%)	14	44
All	All	896/1012 (88%)	838 (94%)	58 (6%)	15	47

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	76	MET
1	A	131	SER
1	A	132	THR
1	A	136	THR
1	A	145	LEU
1	A	214	GLN
1	A	215	LEU
1	A	239	LEU
1	A	240	LEU
1	A	241	LEU
1	A	242	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	264	VAL
1	A	268	ILE
1	B	76	MET
1	B	131	SER
1	B	132	THR
1	B	136	THR
1	B	145	LEU
1	B	214	GLN
1	B	215	LEU
1	B	239	LEU
1	B	240	LEU
1	B	241	LEU
1	B	242	LEU
1	B	264	VAL
1	B	268	ILE
2	C	9	VAL
2	C	11	LEU
2	C	21	VAL
2	C	40	VAL
2	C	83	LEU
2	C	87	ARG
2	C	116	SER
2	C	119	ARG
2	C	122	LEU
2	C	132	LEU
2	C	155	VAL
2	C	175	THR
2	C	205	LEU
2	C	218	ILE
2	C	231	THR
2	C	241	LEU
2	D	11	LEU
2	D	21	VAL
2	D	40	VAL
2	D	83	LEU
2	D	87	ARG
2	D	116	SER
2	D	119	ARG
2	D	122	LEU
2	D	132	LEU
2	D	155	VAL
2	D	175	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	205	LEU
2	D	218	ILE
2	D	231	THR
2	D	241	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	B	6	GLN
2	C	18	HIS
2	C	128	GLN
2	C	158	GLN
2	C	161	GLN
2	D	18	HIS
2	D	128	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	D	301	-	4,4,4	0.98	0	6,6,6	0.57	0
3	PO4	C	301	-	4,4,4	0.59	0	6,6,6	0.73	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	297/357 (83%)	1.19	44 (14%) 5 3	52, 102, 163, 207	0
1	B	297/357 (83%)	0.70	28 (9%) 14 7	74, 110, 176, 215	0
2	C	262/266 (98%)	0.37	12 (4%) 37 20	67, 79, 124, 163	0
2	D	257/266 (96%)	0.61	16 (6%) 26 14	64, 107, 171, 208	0
All	All	1113/1246 (89%)	0.73	100 (8%) 15 8	52, 99, 168, 215	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	233	GLU	7.4
1	B	323	TRP	4.6
1	A	140	TRP	4.6
1	B	140	TRP	4.5
2	D	56	LEU	4.3
1	A	273	GLY	4.1
1	B	273	GLY	4.1
1	A	4	ARG	4.1
1	B	176	ARG	4.1
1	A	180	LEU	4.0
1	A	74	THR	4.0
1	B	326	LEU	4.0
1	A	257	ILE	3.9
2	C	95	GLU	3.8
2	D	116	SER	3.8
1	A	270	MET	3.7
1	A	185	SER	3.7
1	A	165	VAL	3.6
1	A	266	HIS	3.6
1	B	48	TRP	3.6
1	B	177	GLN	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	163	VAL	3.5
1	A	204	THR	3.5
1	A	239	LEU	3.3
2	C	234	GLU	3.3
1	B	180	LEU	3.2
2	D	92	GLN	3.2
1	A	176	ARG	3.1
1	A	91	GLY	3.1
2	D	81	LYS	3.1
1	A	212	ALA	3.1
1	B	301	LEU	3.1
1	A	192	SER	3.1
1	A	120	MET	3.0
1	B	304	PRO	2.9
1	B	322	LEU	2.9
1	B	306	GLU	2.9
2	C	229	CYS	2.9
1	B	175	LEU	2.9
1	A	167	THR	2.8
1	B	320	TYR	2.8
2	D	136	GLN	2.8
1	A	57	PRO	2.8
1	A	145	LEU	2.8
1	A	181	TRP	2.8
1	A	326	LEU	2.8
1	B	143	GLY	2.8
2	D	163	GLN	2.8
1	B	321	PHE	2.7
2	C	22	GLN	2.7
2	C	48	ALA	2.7
1	A	88	GLY	2.6
1	B	258	GLY	2.6
1	B	324	LEU	2.6
2	D	85	ARG	2.6
1	B	56	LEU	2.5
1	A	119	HIS	2.5
2	D	65	HIS	2.5
2	D	175	THR	2.5
2	D	164	PRO	2.5
1	A	252	ALA	2.5
1	A	260	ILE	2.5
2	D	120	GLN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	118	SER	2.4
1	B	179	SER	2.4
1	A	146	ALA	2.4
1	A	306	GLU	2.4
1	A	164	GLY	2.4
1	A	321	PHE	2.4
1	A	61	LEU	2.4
2	C	60	TYR	2.3
2	C	253	ARG	2.3
2	D	72	GLY	2.3
1	A	175	LEU	2.3
2	C	92	GLN	2.3
1	A	116	LEU	2.3
1	B	50	ILE	2.3
1	B	104	ILE	2.3
2	D	25	ALA	2.3
2	D	229	CYS	2.2
2	C	66	GLY	2.2
2	C	46	ASN	2.2
1	A	117	TYR	2.2
2	D	61	LEU	2.2
1	A	278	TRP	2.2
1	B	165	VAL	2.1
2	D	22	GLN	2.1
1	A	65	VAL	2.1
1	A	262	LEU	2.1
1	B	142	HIS	2.1
1	A	322	LEU	2.1
1	A	25	SER	2.0
1	A	179	SER	2.0
1	A	98	LEU	2.0
1	B	4	ARG	2.0
1	B	137	LEU	2.0
2	C	175	THR	2.0
1	B	60	LEU	2.0
1	A	154	ALA	2.0
1	A	20	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	C	301	5/5	0.60	0.28	56,61,80,101	0
3	PO4	D	301	5/5	0.78	0.11	133,135,165,185	0

6.5 Other polymers [i](#)

There are no such residues in this entry.